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NEWS 1	Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	"Ask CAS" for self-help around the clock
NEWS 3 JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4 FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5 FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6 FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7 FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8 MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9 MAR 22	EMBASE is now updated on a daily basis
NEWS 10 APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11 APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12 APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS 13 APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14 APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15 APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16 MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS 17 MAY 11	KOREAPAT updates resume
NEWS 18 MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 19 MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPTFULL/USPAT2
NEWS 20 MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS 21 JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS	FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available after June 2006

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FILE 'HOME' ENTERED AT 18:40:18 ON 21 JUN 2006

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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FILE 'BIOSIS' ENTERED AT 18:40:38 ON 21 JUN 2006

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FILE 'WPIDS' ENTERED AT 18:40:38 ON 21 JUN 2006

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=> e stockman brian?/au

E1	85	STOCKMAN BRIAN J/AU
E2	1	STOCKMAN BRIAN JOHN/AU
E3	0 -->	STOCKMAN BRIAN?/AU
E4	6	STOCKMAN BRONISLAVA M/AU
E5	8	STOCKMAN C/AU
E6	1	STOCKMAN C F/AU
E7	5	STOCKMAN C H/AU
E8	1	STOCKMAN C H J/AU
E9	2	STOCKMAN C R/AU
E10	8	STOCKMAN C T/AU
E11	1	STOCKMAN CAMPBELL K H/AU
E12	1	STOCKMAN CAMPBELL KEITH HENRY/AU

=> e1 or e2

L1 86 "STOCKMAN BRIAN J"/AU OR "STOCKMAN BRIAN JOHN"/AU

=> dup rem l1

PROCESSING COMPLETED FOR L1

L2 61 DUP REM L1 (25 DUPLICATES REMOVED)

=> nmr and l2

L3 52 NMR AND L2

=> library and l3

L4 8 LIBRARY AND L3

=> relax? and l3

L5 6 RELAX? AND L3

=> l4 and l5

L6 1 L4 AND L5

=> d ibib abs 16

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:563654 CAPLUS

DOCUMENT NUMBER: 135:313029

TITLE: Screening of compound libraries for protein binding using flow-injection nuclear magnetic resonance spectroscopy

AUTHOR(S): **Stockman, Brian J.**; Farley, Kathleen A.; Angwin, Daneen T.

CORPORATE SOURCE: Structural, Analytical, and Medicinal Chemistry, Pharmacia Corporation, Kalamazoo, MI, 49001, USA

SOURCE: Methods in Enzymology (2001), 338(Nuclear Magnetic Resonance of Biological Macromolecules, Part A), 230-246

CODEN: MENZAU; ISSN: 0076-6879

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 48 refs on the use of flow-injection **NMR** spectroscopy to screen compound libraries for protein binding. Topics include data acquisition hardware and software; flow probe calibration and system optimization; design of small mol. screening libraries; **relaxation**-edited flow-injection **NMR** screening; data anal.; and comparisons between flow and traditional methods. (c) 2001 Academic Press.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	22.34	22.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 16, 2006 (20060616/UP).

=> fil medline biosis caplus scisearch embase wpids

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.66	23.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

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(FILE 'HOME' ENTERED AT 18:40:18 ON 21 JUN 2006)

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
18:40:38 ON 21 JUN 2006

E STOCKMAN BRIAN?/AU

L1 86 E1 OR E2
L2 61 DUP REM L1 (25 DUPLICATES REMOVED)
L3 52 NMR AND L2
L4 8 LIBRARY AND L3
L5 6 RELAX? AND L3
L6 1 L4 AND L5

FILE 'STNGUIDE' ENTERED AT 18:43:22 ON 21 JUN 2006

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
18:50:10 ON 21 JUN 2006

=> d ibib abs l4 1-8

L4 ANSWER 1 OF 8 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2004:332743 BIOSIS
DOCUMENT NUMBER: PREV200400337451
TITLE: Methods for creating a compound **library**.
AUTHOR(S): **Stockman, Brian J.** [Inventor, Reprint Author]
CORPORATE SOURCE: ASSIGNEE: Pharmacia & Upjohn Company
PATENT INFORMATION: US 6764858 20040720
SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (July 20 2004) Vol. 1284, No. 3.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 4 Aug 2004
Last Updated on STN: 4 Aug 2004

AB A method for developing a **library** of compounds, the compound
library, a method for identifying ligands for target molecules,
and a method for identifying lead chemical templates, which, for example,
can be used in drug discovery and design are provided. Certain
embodiments of these methods include the use of **NMR**
spectroscopy.

L4 ANSWER 2 OF 8 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2004:101827 BIOSIS
DOCUMENT NUMBER: PREV200400104165
TITLE: Methods for creating a compound **library** and
identifying lead chemical templates and ligands for target

molecules.
AUTHOR(S): **Stockman, Brian J.** [Inventor, Reprint Author];
Farley, Kathleen A. [Inventor]; Dalvit, Claudio [Inventor]
CORPORATE SOURCE: Kalamazoo, MI, USA
ASSIGNEE: Pharmacia & Upjohn Company
PATENT INFORMATION: US 6677160 20040113
SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (Jan 13 2004) Vol. 1278, No. 2.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 18 Feb 2004
Last Updated on STN: 18 Feb 2004

AB A method for developing a **library** of compounds, the compound
library, a method for identifying ligands for target molecules,
and a method for identifying lead chemical templates, which, for example,
can be used in drug discovery and design are provided. Certain
embodiments of these methods include the use of **NMR**
spectroscopy.

L4 ANSWER 3 OF 8 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2002:38396 BIOSIS
DOCUMENT NUMBER: PREV200200038396
TITLE: Screening of compound libraries for protein binding using
flow-injection nuclear magnetic resonance spectroscopy.
AUTHOR(S): **Stockman, Brian J.**; Farley, Kathleen A.; Angwin,
Daneen T.
SOURCE: James, Thomas L.; Dotsch, Volker; Schmitz, Uli. Methods
Enzymol., (2001) pp. 230-246. Methods in Enzymology.
Nuclear magnetic resonance of biological macromolecules:
Part A. print.
Publisher: Academic Press Inc., 525 B Street, Suite 1900,
San Diego, CA, 92101-4495, USA; Academic Press Ltd.,
Harcourt Place, 32 Jamestown Road, London, NW1 7BY, UK.
Series: Methods in Enzymology.
CODEN: MENZAU. ISSN: 0076-6879. ISBN: 0-12-182239-7
(cloth).
DOCUMENT TYPE: Book
Book; (Book Chapter)
LANGUAGE: English
ENTRY DATE: Entered STN: 2 Jan 2002
Last Updated on STN: 25 Feb 2002

L4 ANSWER 4 OF 8 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:161682 BIOSIS
DOCUMENT NUMBER: PREV199598175982
TITLE: Chemical shift differences between free and Fab-bound
peptide correlate with a two-stage selection of peptide
sequences from a random phage display **library** to
delineate critical and non-critical residues from antibody
recognition.
AUTHOR(S): **Stockman, Brian J.** [Reprint author]; Bannow,
Carol A.; Miceli, Robert M.; Degraaf, Michael E.; Fischer,
H. David; Smith, Clark W.
CORPORATE SOURCE: Physical Analytical Chem., M/S 7255-209-007, 301 Henrietta
St., Upjohn Co., Kalamazoo, MI 49001, USA
SOURCE: International Journal of Peptide and Protein Research,
(1995) Vol. 45, No. 1, pp. 11-16.
CODEN: IJPPC3. ISSN: 0367-8377.
DOCUMENT TYPE: Article
LANGUAGE: English

ENTRY DATE: Entered STN: 11 Apr 1995
Last Updated on STN: 11 Apr 1995

AB Epitope libraries provide a method to identify peptide ligands for antibodies, receptors or other binding proteins. As such, they provide a powerful tool to rapidly identify lead ligands in the drug discovery process. In an attempt to correlate structural information with the results from peptide screening, we have used **NMR** spectroscopy of peptide/antibody complexes to demonstrate that core residues identified through a two-stage selection process undergo a larger structural change upon binding antibody than do positions in the peptide amenable to a variety of side chains. The model system used was the M2 monoclonal antibody/Flag octapeptide epitope system. We have analyzed two peptides: Ac-Asp-Tyr-Lys-Leu-Gly-Asp-Asp-Leu-NH-2 (peptide 1), which contains several non-core positions randomized, and Ac-Asp-Tyr-Lys-Asp-Asp-Asp-Leu-NH-2 (peptide 2), which closely corresponds to the original Flag sequence. Enrichment of the peptides with ¹⁵N facilitated the investigation by permitting spectral editing of the peptide resonances in the presence of antibody. For peptide 1 the absolute shifts for the free vs. Fab-bound peptide were found to be largest for the amide groups of Asp-1 and Asp-6, in agreement with classification of these residues as critical by the phage display **library** selection process. For peptide 2 the largest absolute shifts were observed for Asp-1 and Asp-4, with the other aspartic acid residues also showing significant but smaller changes.

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:965009 CAPLUS
DOCUMENT NUMBER: 138:33301
TITLE: Methods for creating a compound **library**, and use in drug discovery and design
INVENTOR(S): **Stockman, Brian J.**; Farley, Kathleen A.
PATENT ASSIGNEE(S): Pharmacia & Upjohn, USA
SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U. S. Ser. No. 677,197.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	-----	-----	-----
US 2002192707	A1	20021219	US 2001-44219	20011119
US 6764858	B2	20040720		
US 6677160	B1	20040113	US 2000-677107	20000929
US 2004086948	A1	20040506	US 2003-694385	20031027
PRIORITY APPLN. INFO.:			US 1999-156818P	P 19990929
			US 1999-161682P	P 19991026
			US 2000-192685P	P 20000328
			US 2000-677107	A2 20000929

AB A method for developing a **library** of compds., the compound **library**, a method for identifying ligands for target mols., and a method for identifying lead chemical templates, which, for example, can be used in drug discovery and design are provided. Certain embodiments of these methods include the use of **NMR** spectroscopy.

REFERENCE COUNT: 148 THERE ARE 148 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:894025 CAPLUS
DOCUMENT NUMBER: 139:78071

TITLE: **NMR** screening techniques in drug discovery and drug design
AUTHOR(S): **Stockman, Brian J.**; Dalvit, Claudio
CORPORATE SOURCE: Structural, Analytical & Medicinal Chemistry, Pharmacia, Kalamazoo, MI, 49001, USA
SOURCE: Progress in Nuclear Magnetic Resonance Spectroscopy (2002), 41(3-4), 187-231
CODEN: PNMRA; ISSN: 0079-6565
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review describes the progress in the field of **NMR** (NMR) screening strategies. It provides a phys. and math. basis of the various **NMR** screening techniques and describes examples from the literature where the techniques have been applied to biol. systems. Emphasis will be placed on applications in drug discovery and drug design. A discussion on **NMR** screening **library** design is also included, with particular emphasis on the elegant SHAPES **library** and its applications. The review will conclude with sections on **NMR** screening's impact on chemical and biol., prospects for automation and future directions.

REFERENCE COUNT: 159 THERE ARE 159 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:563654 CAPLUS
DOCUMENT NUMBER: 135:313029
TITLE: Screening of compound libraries for protein binding using flow-injection nuclear magnetic resonance spectroscopy
AUTHOR(S): **Stockman, Brian J.**; Farley, Kathleen A.; Angwin, Daneen T.
CORPORATE SOURCE: Structural, Analytical, and Medicinal Chemistry, Pharmacia Corporation, Kalamazoo, MI, 49001, USA
SOURCE: Methods in Enzymology (2001), 338(Nuclear Magnetic Resonance of Biological Macromolecules, Part A), 230-246
CODEN: MENZAU; ISSN: 0076-6879
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 48 refs on the use of flow-injection **NMR** spectroscopy to screen compound libraries for protein binding. Topics include data acquisition hardware and software; flow probe calibration and system optimization; design of small mol. screening libraries; relaxation-edited flow-injection **NMR** screening; data anal.; and comparisons between flow and traditional methods. (c) 2001 Academic Press.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:247291 CAPLUS
DOCUMENT NUMBER: 134:261221
TITLE: Methods for creating a compound **library** and identifying lead chemical templates and ligands for target molecules
INVENTOR(S): **Stockman, Brian J.**; Farley, Kathleen
PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023330	A2	20010405	WO 2000-US41034	20000929
WO 2001023330	A3	20020510		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2400094	AA	20010405	CA 2000-2400094	20000929
AU 2001014944	A5	20010430	AU 2001-14944	20000929
EP 1242339	A2	20020925	EP 2000-977289	20000929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRIORITY APPLN. INFO.:			US 1999-156818P	P 19990929
			US 1999-161682P	P 19991026
			US 2000-192685P	P 20000328
			WO 2000-US41034	W 20000929

AB A method for developing a **library** of compds., the compound **library**, a method for identifying ligands for target mols., and a method for identifying lead chemical templates, which, for example, can be used in drug discovery and design, are provided. Certain embodiments of these methods include the use of **NMR** spectroscopy.

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	30.52	53.73
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CA SUBSCRIBER PRICE	-3.00	-3.75

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FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Jun 16, 2006 (20060616/UP).

=> fil medline biosis caplus scisearch embase wpids

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FULL ESTIMATED COST	0.60	54.33
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.75

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=> d ibib abs 15 1-6

L5 ANSWER 1 OF 6 MEDLINE on STN
ACCESSION NUMBER: 2002708835 MEDLINE
DOCUMENT NUMBER: PubMed ID: 12470257
TITLE: Fluorine-**NMR** competition binding experiments for
high-throughput screening of large compound mixtures.
AUTHOR: Dalvit Claudio; Flocco Maria; Veronesi Marina;
Stockman Brian J
CORPORATE SOURCE: Chemistry Department, Pharmacia, Viale Pasteur 10, Nerviano
(MI), 20014, Italy.. claudio.dalvit@pharmacia.com
SOURCE: Combinatorial chemistry & high throughput screening, (2002
Dec) Vol. 5, No. 8, pp. 605-11.
Journal code: 9810948. ISSN: 1386-2073.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200301
ENTRY DATE: Entered STN: 17 Dec 2002
Last Updated on STN: 11 Jan 2003
Entered Medline: 10 Jan 2003

AB High-throughput ligand-based **NMR** screening with competition
binding experiments is extended to (19)F detection. Fluorine is a
favorable nucleus for these experiments because of the significant
contribution of the Chemical Shift Anisotropy (CSA) to the (19)F
transverse **relaxation** of the ligand signal when bound to a
macromolecular target. A low to moderate affinity ligand containing a
fluorine atom is used as a reference molecule for the detection and
characterization of new ligands. Titration **NMR** experiments with
the selected reference compound are performed for finding the optimal
set-up conditions for HTS and for deriving the binding constants of the
identified **NMR** hits. Rapid HTS of large chemical mixtures and
plant or fungi extracts against the receptor of interest is possible due
to the high sensitivity of the (19)F nucleus and the absence of overlap
with the signals of the mixtures to be screened. Finally, a novel
approach for HTS using a reference molecule in combination with a control
molecule is presented.

L5 ANSWER 2 OF 6 MEDLINE on STN
ACCESSION NUMBER: 2002342083 MEDLINE
DOCUMENT NUMBER: PubMed ID: 12083923
TITLE: High-throughput **NMR**-based screening with
competition binding experiments.
AUTHOR: Dalvit Claudio; Flocco Maria; Knapp Stefan; Mostardini

Marina; Perego Rita; **Stockman Brian J**; Veronesi
 Marina; Varasi Mario
 CORPORATE SOURCE: Chemistry Department, Pharmacia, Viale Pasteur 10, 20014
 Nerviano (MI), Milan, Italy.. claudio.dalvit@pharmacia.com
 SOURCE: Journal of the American Chemical Society, (2002 Jul 3) Vol.
 124, No. 26, pp. 7702-9.
 Journal code: 7503056. ISSN: 0002-7863.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200208
 ENTRY DATE: Entered STN: 27 Jun 2002
 Last Updated on STN: 14 Aug 2002
 Entered Medline: 13 Aug 2002

AB The Achilles heel of ligand-based **NMR** screening methods is their failure to detect high-affinity ligands and molecules that bind covalently to the receptor. We have developed a novel approach for performing high-throughput screening with **NMR** spectroscopy that overcomes this limitation. The method also permits detection of potential high-affinity molecules that are only marginally soluble, thus significantly enlarging the diversity of compounds amenable to **NMR** screening. The techniques developed utilize transverse and/or selective longitudinal **relaxation** parameters in combination with competition binding experiments. Mathematical expressions are derived for proper setup of the **NMR** experiments and for extracting an approximate value of the binding constant for the identified ligand from a single-point measurement. With this approach it is possible to screen thousands of compounds in a short period of time against protein or DNA and RNA fragments. The methodology can also be applied for screening plant and fungi extracts.

L5 ANSWER 3 OF 6 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
 ACCESSION NUMBER: 2000:8482 BIOSIS
 DOCUMENT NUMBER: PREV200000008482
 TITLE: Dynamics of stromelysin/inhibitor interactions studied by
 15N **NMR relaxation** measurements:
 Comparison of ligand binding to the S1-S3 and S1'-S3'
 subsites.
 AUTHOR(S): Yuan, Peng; Marshall, Vincent P.; Petzold, Gary L.;
 Poorman, Roger A.; **Stockman, Brian J.** [Reprint
 author]
 CORPORATE SOURCE: Structural, Analytical and Medicinal Chemistry and Protein
 Science, Pharmacia and Upjohn, 301 Henrietta St.,
 Kalamazoo, MI, 49001, USA
 SOURCE: Journal of Biomolecular NMR, (Sept., 1999) Vol. 15, No. 1,
 pp. 55-64. print.
 CODEN: JBNME9. ISSN: 0925-2738.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 23 Dec 1999
 Last Updated on STN: 31 Dec 2001

AB This report describes the backbone amide dynamics of the uniformly 15N labeled catalytic domain of human stromelysin complexed to PNU-99533, a hydroxamate-containing ligand that binds to the S1'-S3' region (right side) of the stromelysin active site, and to PNU-107859 and PNU-142372, both thiadiazole-containing ligands that bind to the S1-S3 region (left side) of the stromelysin active site. 15N R1, R2 and NOE **NMR relaxation** measurements were recorded and analyzed for each complex. Different dynamic behaviors were observed for stromelysin complexed to the two classes of ligands, indicating that it may be possible to use protein dynamics to distinguish between different binding

orientations. In the absence of bound ligand at the S1-S3 subsites, the S1-S3 residues were found to be relatively rigid. In contrast, the S1'-S3' subsites were found to be flexible in the absence of interactions with ligand. The relative rigidity of the S1-S3 subsites may be responsible for MM P binding specificity by discriminating between ligands of different shapes. By contrast, the inherent flexibility of the S1'-S3' subsites allows structural rearrangement to accommodate a broad range of incoming substrates or inhibitors. Similarities and differences in dynamics observed for each complex provide insights into the interactions responsible for protein-ligand recognition. The relevance of protein dynamics to structure-based drug design is discussed.

L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:982940 CAPLUS

TITLE: Competition-Based **Nmr** Binding Assays

AUTHOR(S): **Stockman, Brian J.**

CORPORATE SOURCE: Groton Laboratories, Pfizer Inc., Groton, CT, 06340, USA

SOURCE: Abstracts, 56th Southeast Regional Meeting of the American Chemical Society, Research Triangle Park, NC, United States, November 10-13 (2004), GEN-302. American Chemical Society: Washington, D. C. CODEN: 69FWAQ

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Traditional ligand-observed **NMR** binding expts. are restricted to ligands with good aqueous solubility and are limited to the identification of ligands having target affinities in the M to mM range. Recently introduced competition-based **NMR** binding assays overcome these limitations and allow ligands with marginal aqueous solubility and target affinities in the nM range to be identified. Competition-based **NMR** binding assays utilizing WaterLOGSY, longitudinal **relaxation**, and transverse **relaxation** methods will be described. WaterLOGSY and longitudinal **relaxation** methods utilize ¹H detection. Transverse **relaxation** methods can utilize either ¹H or ¹⁹F detection. The advantages of ¹⁹F detection, including high sensitivity and reduced spectral overlap, will be discussed.

L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:563654 CAPLUS

DOCUMENT NUMBER: 135:313029

TITLE: Screening of compound libraries for protein binding using flow-injection nuclear magnetic resonance spectroscopy

AUTHOR(S): **Stockman, Brian J.**; Farley, Kathleen A.; Angwin, Daneen T.

CORPORATE SOURCE: Structural, Analytical, and Medicinal Chemistry, Pharmacia Corporation, Kalamazoo, MI, 49001, USA

SOURCE: Methods in Enzymology (2001), 338 (Nuclear Magnetic Resonance of Biological Macromolecules, Part A), 230-246

CODEN: MENZAU; ISSN: 0076-6879

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 48 refs on the use of flow-injection **NMR** spectroscopy to screen compound libraries for protein binding. Topics include data acquisition hardware and software; flow probe calibration and system optimization; design of small mol. screening libraries; **relaxation**-edited flow-injection **NMR** screening; data anal.; and comparisons between flow and traditional methods. (c) 2001 Academic Press.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:231124 CAPLUS
DOCUMENT NUMBER: 116:231124
TITLE: **NMR** studies of structure and dynamics of isotope enriched proteins
AUTHOR(S): Wagner, Gerhard; Thanabal, V.; **Stockman, Brian J.**; Peng, Jeffrey W.; Nirmala, N. R.; Hyberts, Sven G.; Goldberg, Matthew S.; Detlefsen, David J.; Clubb, Robert T.; Adler, Marc
CORPORATE SOURCE: Dep. Biol. Chem. Mol. Pharmacol., Harvard Med. Sch., Boston, MA, 02115, USA
SOURCE: Biopolymers (1992), 32(4), 381-90
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Structural studies of globular proteins by **NMR** can be enhanced by isotope enrichment with ¹⁵N, and with both ¹⁵N and ¹³C. Using these techniques, several large proteins with up to 186 residues were assigned and structural questions addressed. Furthermore, heteronuclear and homonuclear vicinal coupling consts. were accurately measured. This involves in part multidimensional multiple resonance expts. This is important for characterization of minor conformational changes caused by mutations. Isotope enrichment was also used to study the internal mobility of proteins. Novel methods for measuring accurately ¹⁵N **relaxation** parameters, in particular transverse **relaxation** rates were also developed. This has led toward a method for directly mapping spectral d. functions of the rotational motions of N-H bond vectors in proteins. The protein system discussed include the unlabeled proteins kistrin and cytochrome c551, and the labeled proteins elgin c, a flavodoxin, and human dihydrofolate reductase.

=> relax? and nmr

L7 67575 RELAX? AND NMR

=> library and inject? and ((multi or 96) (w) well) and l7

L8 0 LIBRARY AND INJECT? AND ((MULTI OR 96) (W) WELL) AND L7

=> library and inject? and l7

L9 2 LIBRARY AND INJECT? AND L7

=> dup rem l9

PROCESSING COMPLETED FOR L9

L10 2 DUP REM L9 (0 DUPLICATES REMOVED)

=> d ibib abs l10 1-2

L10 ANSWER 1 OF 2 WPIDS COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2001-300093 [31] WPIDS
DOC. NO. NON-CPI: N2001-215345
DOC. NO. CPI: C2001-092085
TITLE: Methods for creating a compound **library** and identifying lead chemical templates and ligands for target molecules by comparing **NMR** spectra of a mixture in the presence of a target molecule with those obtained without the target molecule.
DERWENT CLASS: B04 J04 S02 S03
INVENTOR(S): FARLEY, K; STOCKMAN, B J; FARLEY, K A; DALVIT, C
PATENT ASSIGNEE(S): (PHAA) PHARMACIA & UPJOHN CO; (PHAA) PHARMACIA & UPJOHN

COUNTRY COUNT: 95
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2001023330	A2	20010405	(200131)*	EN	61
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TZ UG ZW					
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CR CU CZ DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW					
AU 2001014944	A	20010430	(200142)		
EP 1242339	A2	20020925	(200271)	EN	
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL RO SI					
US 2002192707	A1	20021219	(200303)		
US 6677160	B1	20040113	(200405)		
US 2004086948	A1	20040506	(200430)		
US 6764858	B2	20040720	(200448)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001023330	A2	WO 2000-US41034	20000929
AU 2001014944	A	AU 2001-14944	20000929
EP 1242339	A2	EP 2000-977289	20000929
		WO 2000-US41034	20000929
US 2002192707	A1 Provisional	US 1999-156818P	19990929
	Provisional	US 1999-161682P	19991026
	Provisional	US 2000-192685P	20000328
	CIP of	US 2000-677107	20000929
		US 2001-44219	20011119
US 6677160	B1 Provisional	US 1999-156818P	19990929
	Provisional	US 1999-161682P	19991026
	Provisional	US 2000-192685P	20000328
		US 2000-677107	20000929
US 2004086948	A1 Provisional	US 1999-156818P	19990929
	Provisional	US 1999-161682P	19991026
	Provisional	US 2000-192685P	20000328
	Div ex	US 2000-677107	20000929
		US 2003-694385	20031027
US 6764858	B2 Provisional	US 1999-156818P	19990929
	Provisional	US 1999-161682P	19991026
	Provisional	US 2000-192685P	20000328
	CIP of	US 2000-677107	20000929
		US 2001-44219	20011119

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001014944	A Based on	WO 2001023330
EP 1242339	A2 Based on	WO 2001023330
US 2004086948	A1 Div ex	US 6677160

PRIORITY APPLN. INFO: US 2000-192685P 20000328; US
1999-156818P 19990929; US
1999-161682P 19991026; US
2000-677107 20000929; US
2001-44219 20011119; US

2003-694385

20031027

AN 2001-300093 [31] WPIDS

AB WO 200123330 A UPAB: 20010607

NOVELTY - A method of creating a chemical compound **library** comprises selecting compounds having a molecular weight of no more than 350Da and a solubility in deuteriated water of at least 1mM at room temperature.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for

(i) a chemical compound **library** comprising compounds having a molecular weight of no more than 350Da and a solubility in deuteriated water of at least 1mM at room temperature;

(ii) a method of identifying a lead chemical template comprising identifying compounds from the **library** that function as a ligand to a target molecule having a dissociated constant of at least 100 μ M and using the ligand to identify a lead chemical template;

(iii) a method of identifying a compound that binds to a target molecule comprising comparing **relaxation**-edited **NMR** spectra obtained from a flow-**injection** probe of a mixture of test compounds in the presence of a target molecule with the spectrum obtained without the target compound;

(iv) a method of identifying a compound that binds to a target molecule comprising analyzing WaterLOGSY **NMR** spectra obtained from a flow-**injection** probe of a mixture of test compounds in the presence of a target molecule to distinguish binding compounds from non-binding compounds by virtue of the opposite sign of their water-ligand nOe 's.

USE - The method is useful for creating a compound **library** and identifying lead chemical templates and ligands for target molecules.
Dwg.0/16

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:563654 CAPLUS

DOCUMENT NUMBER: 135:313029

TITLE: Screening of compound libraries for protein binding using flow-**injection** nuclear magnetic resonance spectroscopy

AUTHOR(S): Stockman, Brian J.; Farley, Kathleen A.; Angwin, Daneen T.

CORPORATE SOURCE: Structural, Analytical, and Medicinal Chemistry, Pharmacia Corporation, Kalamazoo, MI, 49001, USA

SOURCE: Methods in Enzymology (2001), 338 (Nuclear Magnetic Resonance of Biological Macromolecules, Part A), 230-246

CODEN: MENZAU; ISSN: 0076-6879

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 48 refs on the use of flow-**injection NMR** spectroscopy to screen compound libraries for protein binding. Topics include data acquisition hardware and software; flow probe calibration and system optimization; design of small mol. screening libraries; **relaxation**-edited flow-**injection NMR** screening; data anal.; and comparisons between flow and traditional methods. (c) 2001 Academic Press.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 18:40:18 ON 21 JUN 2006)

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
18:40:38 ON 21 JUN 2006

E STOCKMAN BRIAN?/AU

L1 86 E1 OR E2
L2 61 DUP REM L1 (25 DUPLICATES REMOVED)
L3 52 NMR AND L2
L4 8 LIBRARY AND L3
L5 6 RELAX? AND L3
L6 1 L4 AND L5

FILE 'STNGUIDE' ENTERED AT 18:43:22 ON 21 JUN 2006

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
18:50:10 ON 21 JUN 2006

FILE 'STNGUIDE' ENTERED AT 18:53:04 ON 21 JUN 2006

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
18:59:01 ON 21 JUN 2006

L7 67575 RELAX? AND NMR
L8 0 LIBRARY AND INJECT? AND ((MULTI OR 96) (W) WELL) AND L7
L9 2 LIBRARY AND INJECT? AND L7
L10 2 DUP REM L9 (0 DUPLICATES REMOVED)

=> logoff y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
53.85	108.18

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-3.00	-6.75

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